Role of excited states in the splitting dynamics of interacting Bose-Einstein condensates when ramping-up a barrier

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Abstract

An essentially-exact approach to compute the wavefunction in the time-dependent many-boson Schrödinger equation is derived and employed to study accurately the process of splitting a trapped condensate when ramping-up a barrier such that a double-well is formed. We follow the role played by many-body excited states during the splitting process. Among others, a 'counter-intuitive' regime is found in which the evolution of the condensate when the barrier is ramped-up sufficiently slow *is not* to the ground-state which is a fragmented condensate, but to a low-lying excited-state which is a coherent condensate. Experimental implications are discussed.

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The first realizations of Bose-Einstein condensate in ultra-cold dilute gases have boosted the community to explore matter-wave phenomena and how to manipulate and utilize them. An ultimate goal of researchers is to be able to design, realize and detect a desired quantum state of the many-atom system. One of the most popular 'screenplays' studied is splitting of Bose-Einstein condensates (BECs) by deforming a single well to a double-well, see [1, 2, 3, 4, 5] for experimental and [6, 7, 8, 9, 10, 11] for theoretical works. In such scenarios, the many-atom system is often prepared in the ground-state of a harmonic trap and a central barrier is ramped-up to a certain fixed height. As the trap transforms from harmonic to double-well geometry the time-dependent state of the many-boson system continuously changes its localization from the center of the initial trap to two separated parts localized around the minima of the double-well. Side by side, it can also change its character – from condensed to a two-fold fragmented state [8]. Attacking the splitting process, much attention has been paid to understanding when it is adiabatic [6, 7, 8], demonstrating that the slower the barrier is ramped-up (to a certain fixed height), the closer is the BEC to the ground-state of the bosons in the double-well.

In the present work we study the dynamics of splitting when ramping-up a barrier beyond the presently available theoretical and computational approaches. We develop and report on an essentially-exact and numerically-efficient approach for the solution of the time-dependent many-boson Schrödinger equation, which we term multi-configurational time-dependent Hartree for bosons (MCTDHB). Applying MCTDHB to the ramping-up-a-barrier problem we follow the many-boson wavefunction throughout the splitting process and identify the role and impact of many-body *excited-states* on the splitting process. Among others, we identify a new 'counter-intuitive' regime where the evolution of the condensate when the barrier in ramped-up sufficiently slow *is not* to the ground-state of the double-well which is a fragmented BEC, but to a low-lying excited-state which is a coherent BEC. More details are given below.

Our starting point is the many-body Hamiltonian describing N interacting bosons in a trap, $\hat{H} = \sum_{k=1}^{N}\left[\hat{T}(\mathbf{r}_k) + V(\mathbf{r}_k, t)\right] + \sum_{k>l=1}^{N} U(\mathbf{r}_k - \mathbf{r}_l)$. Here, $\mathbf{r}_k$ is the coordinate of the k-th particle, $\hat{T}(\mathbf{r})$ and $V(\mathbf{r}, t)$ stand for the kinetic energy and trap potential, respectively, and $U(\mathbf{r}_k - \mathbf{r}_l)$ describes the pairwise interaction between the k-th and l-th atoms. To solve the time-dependent Schrödinger equation $\hat{H}\Psi = i\frac{\partial\Psi}{\partial t}$ we write the many-body wavefunction

Ψ as a linear combination of *time-dependent* permanents

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) = \sum_{\vec{n}} C_{\vec{n}}(t) \Phi_{\vec{n}}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t). \tag{1}$$

In the representation (1), the time-dependent permanents $\Phi_{\vec{n}}$ are constructed by distributing the N bosons over $j = 1, \ldots, M$ *time-dependent* one-particle functions (orbitals) $\{\phi_j(\mathbf{r}, t)\}$, and the summation runs over all possible occupations $\vec{n}$ preserving the total number of bosons N.

To proceed, we utilize the Dirac-Frenkel variational principle [12] and after some lengthy but straightforward algebra obtain a set of coupled non-linear, generally integro-differential equations for the coefficients $C_{\vec{n}}(t)$ and orbitals $\{\phi_j(\mathbf{r}, t)\}$, for all $\vec{n}$ and $j = 1, \ldots, M$,

$$\hat{\mathbf{P}} \left[\left\{ \hat{T}(\mathbf{r}) + V(\mathbf{r}, t) \right\} \phi_j(\mathbf{r}, t) + \sum_{qksl} \{\boldsymbol{\rho}(t)\}^{-1}_{jq} \, \rho_{qksl}(t) U_{kl}(\mathbf{r}, t) \phi_s(\mathbf{r}, t) \right] = i \frac{\partial \phi_j(\mathbf{r}, t)}{\partial t},$$

$$\sum_{\vec{n}'} \left\langle \Phi_{\vec{n}} \left| \hat{H} \right| \Phi_{\vec{n}'} \right\rangle C_{\vec{n}'}(t) = i \frac{dC_{\vec{n}}(t)}{dt}. \tag{2}$$

The quantities $\boldsymbol{\rho}(t) = \{\rho_{qs}(t)\}$ and $\rho_{qksl}(t)$ appearing in (2) are the matrix elements of the reduced one- and two-body densities of Ψ, $\rho(\mathbf{r}_1|\mathbf{r}'_1; t) = \sum_{qs}^{M} \rho_{qs}(t) \phi^*_q(\mathbf{r}'_1, t) \phi_s(\mathbf{r}_1, t)$ and $\rho(\mathbf{r}_1\mathbf{r}_2|\mathbf{r}'_1, \mathbf{r}'_2; t) = \sum_{qksl}^{M} \rho_{qksl}(t) \phi^*_q(\mathbf{r}'_1, t) \phi^*_k(\mathbf{r}'_2, t) \phi_s(\mathbf{r}_1, t) \phi_l(\mathbf{r}_2, t)$, respectively. The local time-dependent potentials $U_{kl}(\mathbf{r}, t) = \int \phi^*_k(\mathbf{r}', t) U(\mathbf{r} - \mathbf{r}') \phi_l(\mathbf{r}', t) d\mathbf{r}'$ originate from the two-body interaction. Finally, the operator $\hat{\mathbf{P}} = 1 - \sum_{k=1}^{M} |\phi_k(\mathbf{r}, t)\rangle\langle \phi_k(\mathbf{r}, t)|$ appearing on the left-hand-side of Eq. (2) is a projection operator which ensures that the orbitals remain orthogonal to one another throughout the propagation in time [13].

The MCTDHB theory gathered in Eqs. (1,2) is capable by construction to describe the evolution of N-bosons' wavefunctions and thus many-body properties of BECs in time-dependent potentials, and is an essentially-exact time-dependent theory. We stress that it derives from a full, time-dependent variational principle where no restrictions except of orthonormality on the coefficients $C_{\vec{n}}(t)$ and orbitals $\{\phi_j(\mathbf{r}, t)\}$ are employed. The key idea behind expansion (1) is that, by allowing *both* the expansion coefficients $C_{\vec{n}}(t)$ and orbitals $\{\phi_j(\mathbf{r}, t)\}$ used to construct the permanents to be *time-dependent*, a significant computational advantage in solving the many-body Schrödinger equation arises in comparison to many-body expansions with orbitals of fixed shape, also see below. It is gratifying to mention that the present many-body propagation theory adapts to identical bosons the multi-configurational time-dependent Hartree approach routinely used for multi-dimensional dy-

namical systems consisting of distinguishable particles [14]. By explicitly exploiting bosons' statistics it is possible to successfully and quantitatively attack the dynamics of a large number of bosons with the present theory [13]. Finally, we can also propagate the MCTDHB equations (2) in imaginary time and compute for static (time-independent) traps self-consistent ground and excited eigenstates of bosonic systems, since in that case (2) boil down to the general variational many-body theory for interacting bosons developed recently in [15].

Let us study now the splitting dynamics of a repulsive bosonic system from an initial harmonic trap where the ground eigenstate is a slightly depleted condensed state, to the final double-well potential where the ground-state many-body wavefunction is (totally) two-fold fragmented. Specifically, we consider $N = 200$ ^{87}Rb atoms initially prepared in an elongated, quasi-one-dimensional harmonic trap of longitudinal $\omega_{\|} = 2\pi \times 44.7$Hz and transverse $\omega_{\perp} = 2\pi \times 1.1$kHz frequencies. At time $t = 0$ a barrier of Gaussian shape is ramped-up linearly in time to a height of V_{max} and with ramp-up time of T_{ramp}. Introducing a convenient length scale of $L = 1\mu$m, we translate to dimensionless units in which the kinetic energy reads $\hat{T}(x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}$, the time-dependent trap potential is $V(x,t) = \frac{x^2}{2\sigma^2} + V_{max}\exp\left(-\frac{x^2}{2\sigma^2}\right) \times \{t/T_{ramp},\ t \leq T_{ramp}; 1,\ t > T_{ramp}\}$, and the effective atom-atom interaction is $U(x-x') = \lambda_0\delta(x-x')$ where the transverse confinement is properly accounted for [16]. The values of the parameters are $\sigma = 2.6$ and $V_{max} = 30$, corresponding to an inter-well separation of $13.6\mu m$ at the end of the ramping-up process, and $\lambda_0 = 0.1$. Finally, time is expressed in units of $\frac{mL^2}{\hbar} = 1.37$msec, where m is the mass of ^{87}Rb atom, and energy in units of $\frac{\hbar^2}{mL^2} = 116$Hz.

We begin our investigations by ramping-up the barrier during a time of $T_{ramp} = 1000$ until the final double-well is achieved. The developed MCTDHB method is used to solve the time-dependent many-body Schrödinger equation during and following the ramping-up process. Since visualization of the time-dependent many-body wavefunction is quite cumbersome, we prescribe its natural occupation numbers, i.e., eigenvalues of the corresponding reduced one-particle density $\rho(x|x';t) = \sum_j^M \rho_j(t)\phi_j^{*NO}(x',t)\phi_j^{NO}(x,t)$, at each point in time [8, 15]. We have found that for the range of parameters considered here, MCTDHB with two orbitals accurately describes the time-dependent many-body splitting dynamics. The corresponding natural occupation numbers $\rho_1(t)$ and $\rho_2(t)$ are plotted in Fig. 1A as a function of time. The initial state is a slightly depleted condensed state (0.38%) because at $t = 0$ only one natural orbital is macroscopically occupied. As the barrier is ramped-up, $\rho_2(t)$ increases with time,

i.e., the many-body wavefunction becomes more and more depleted. At approximately one third of the ramping-up time $\rho_1(t) = \rho_2(t)$, indicating that the system is momentarily two-fold fragmented. From now on and although the barrier is ramped-up further, the occupation numbers oscillate around this totally fragmented configuration, as has been obtained in [8]. It is worth noticing, however, that an oscillatory behavior of the occupation numbers exists during all the splitting process with different amplitudes and frequencies, see Fig. 1A.

To get a deeper insight into the physics of these oscillations we compute via imaginary time propagation of MCTDHB several low-lying many-body eigenstates of the static system at different barrier heights along the ramping-up path. The energy gap ΔE between the many-body ground- and first excited-state is plotted in Fig. 1B as a function of barrier height. Since the height of the barrier increases linearly with time we can measure the evolution in the units of either ramping-up times or barrier heights. We show that the oscillation frequency of the natural orbitals' occupations can be attributed to ΔE. We define local excitation times $T_{local} = \frac{2\pi}{\Delta E}$ and compare them with the corresponding oscillation periods at different barrier heights.

Here we present a comparison at two different points in time: at $t_I = 0.14T_{ramp}$ and $t_{II} = T_{ramp}$. In the inset of Fig. 1A we plot on an enlarged scale the oscillations of the natural occupation numbers around t_I. The period of oscillations deduced from this inset is $T_I = 13.7$. Since the ramping-up process is linear, t_I corresponds to the barrier height of $V_I = 0.14V_{max}$. The corresponding energy gap $\Delta E_I = 0.47$ gives the value of the local excitation time $T_{local} = \frac{2\pi}{\Delta E_I} = 13.4$, which is close to the observed oscillation period of the natural orbitals for this time-point. Analogously, at t_{II} the observed oscillation period of $T_{II} = 317.9$ agrees with the respective local excitation time of $T_{local} = 333.5$ obtained from the energy gap of $\Delta E_{II} = 0.0188$. We obtain reasonable agreement between corresponding local excitation times and oscillation periods for other times as well. These results can readily be explained: the initial state is the ground-state and the ramping-up process studied is quite slow, implying that at each time-point the propagated state is quite close to the corresponding ground-state. This observation also indicates an adiabatic character of the studied ramping-up process, and that only one many-body excited-state is primarily involved in the dynamics.

Let us now analyze the amplitudes of the oscillations of the natural orbitals. From Fig. 1A we see that oscillations are very modest at the beginning of the ramping-up process

and substantial at the end of the process (notice the logarithmic scale). This is in accord with the decreasing energy gap between the ground and first excited states depicted in Fig. 1B. As expected, an ideal adiabatic ramping-up along the ground-state trajectory is favored by a large energy gap ΔE. It is achieved for ramping-up times T_{ramp} large compared to the local excitation time $T_{local} = \frac{2\pi}{\Delta E}$.

To study quantitatively the adiabatic character of the ramping-up process, we repeat the computation for several different durations of the ramping-up process. The results for $T_{ramp} = 25, 3000, 10000$ are presented in Fig. 2. From this figure a significant suppression of the amplitudes of the oscillations with growing ramping-up times is clearly seen. For the studied system of $N = 200$ bosons, a ramping-up procedure as long as of $T_{ramp} = 10000 =$ 13.7sec still leads to 10.7% fluctuations of the final state. We see that even for such a long ramping-up time, which is of the order of the lifetime of a condensate [5], the final state deviates noticeably from the respective eigenstate and the ramping-up process is still away from being "ideal adiabatic".

In the above example the properties of the ground state and lowest excited state change smoothly with barrier height. For small barrier heights these states are condensed, the excited state being more depleted than the ground state. As the barrier grows, these states become two-fold fragmented and the first excited state results from the ground state by a transfer of a boson from one fragment to another. However, this simple scenario can vary strongly with the number of particles and with their interaction strength [15].

To proceed, we consider the same experiment as before, but with a three-times stronger interaction strength $\lambda_0 = 0.3$. This is achieved by a tighter confinement of $\omega_\perp = 2\pi \times 3.3$kHz. Again, the ground state of the final double-well for this system is fully two-fold fragmented. In Fig. 3A we plot $\rho_1(t)$ and $\rho_2(t)$ for the durations $T_{ramp} = 75$ and $T_{ramp} = 500$ of the ramping-up process. In both cases, the initial wavefunction is the ground eigenstate in the harmonic trap which is a slightly (0.68%) depleted condensed state, see Fig. 3 at $t = 0$. The evolution of $\rho_1(t)$ and $\rho_2(t)$ for the faster ramping-up process of $T_{ramp} = 75$ looks like the "adiabatic" dynamics studied in the previous example but it is not such a dynamics. Indeed, prolonging the ramping-up time, e.g., to $T_{ramp} = 500$, the time-dependent solution does not at all evolve towards the fragmented ground state, but rather to an intermediate state which, according to the occupation number analysis, remains condensed all the time.

To arrive at a deeper insight into the physics behind this 'counter-intuitive' regime, which

we call *inverse* regime, we again investigate the lowest eigenstates of the static double-wells at different barrier heights corresponding to different ramping-up times. The relevant map of static energy gaps ΔE is plotted in Fig. 3B as a function of barrier height. This map has very interesting features – around some critical barrier height $V_{cr} \approx 0.41 V_{max}$ the ground state and lowest excited state come very close to each other and interchange their order. Such a behavior signifying a very narrow avoided crossing (the width of which we cannot detect here) can appear only between states of very different physical origin. Indeed, at $V = 0.40 V_{max}$, the ground state is a slightly depleted condensed state $\rho_1 = 98.14\%$, $\rho_2 = 1.86\%$ while the first excited is almost a totally two-fold fragmented state: $\rho_1 = 51.0\%$, $\rho_2 = 49.0\%$. At $V = 0.42 V_{max}$ we observe an inverse situation: the ground state is now two-fold fragmented $\rho_1 = 50.32\%$, $\rho_2 = 49.68\%$, while the first excited state is condensed $\rho_1 = 98.12\%$, $\rho_2 = 1.88\%$.

The following picture of the ramping-up-a-barrier process emerges in the inverse regime. For a slow ramping-up process, only one quantum eigenstate is essentially populated although another state is crossing or very close by. Clearly, because of the very different physical nature of both states, the initially populated state cannot abruptly change its properties during the relevant time interval and the presence of the partner state essentially does not influence the dynamics. On the other hand, for a faster ramping-up process, more excited eigenstates are involved in the evolution of the many-body wave-function and a coupling between these eigenstates allows the system to overcome the crossing point and evolve towards the lowest eigenstate which is a true two-fold fragmented ground state.

Let us briefly summarize. We show that the dynamics of splitting of an ultra-cold bosonic cloud by ramping-up a barrier depends on the duration of the process and on the (effective) interaction strength between the bosons. There are (at least) two distinct regimes: (i) an *adiabatic* regime where the initial condensed ground-state evolves towards the ground two-fold fragmented eigenstate of the final double-well potential and asymptotically approaches it with increasing ramping-up time; (ii) an *inverse* regime where the initial condensed state evolves towards the ground two-fold fragmented eigenstate only for short ramping-up times, while for slow ramping-up processes the time-dependent state stays condensed during all the evolution and thereby evolves to a *non*-ground many-body eigenstate. The physical insight on these regimes follows from the analysis of the low-lying many-body excited-states taken at different times. The above findings were made possible by developing a multi-

configurational time-dependent Hartree theory for bosons (MCTDHB) capable of providing a quantitative description of the time evolution of the bosonic systems. MCTDHB opens up further possibilities to explore the challenging many-body dynamics of many-boson systems.

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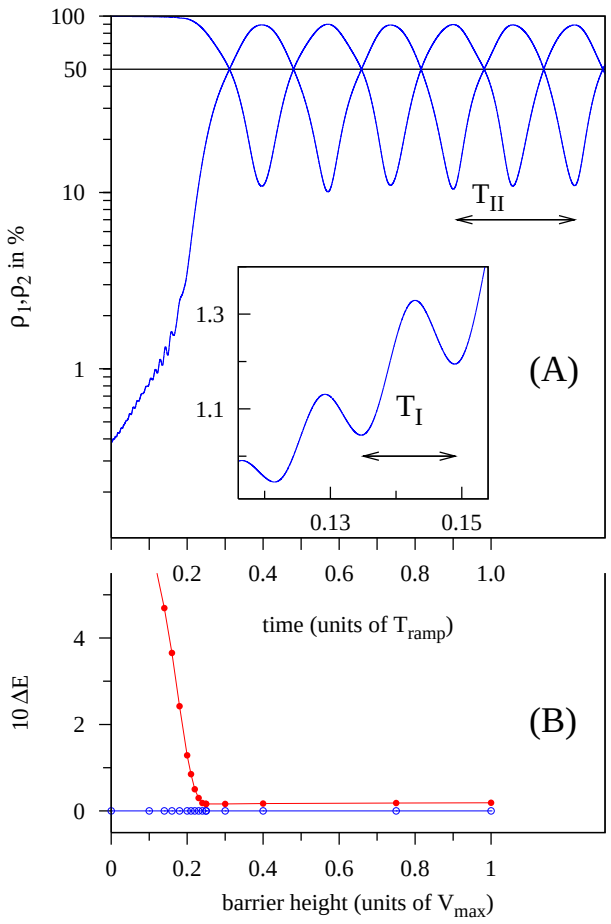

FIG. 1: (Color online) Ramping-up a barrier for $N = 200$ bosons (^{87}Rb atoms) with $\lambda_0 = 0.1$ and ramping-up time $T_{ramp} = 1000$. During the ramping-up process the many-body wavefunction evolves from a condensed towards two-fold fragmented state. (A) Natural occupation numbers $\rho_1(t)$ and $\rho_2(t)$ evaluated at each time-point are plotted on a logarithmic scale. Inset shows oscillatory behavior of the occupation numbers around $t_I = 0.14T_{ramp}$. Periods of the oscillations are attributed to local excitation times, $T_{local} = \frac{2\pi}{\Delta E}$, see text for more details. (B) Energy gap ΔE between the many-body ground- and first excited-state computed as a function of barrier height corresponding to different time-points of the time-dependent trap potential $V(x,t)$. The energy of the ground state is taken as reference energy. Time is expressed in units of $\frac{mL^2}{\hbar} = 1.37$msec and energy in units of $\frac{\hbar^2}{mL^2} = 166$Hz.

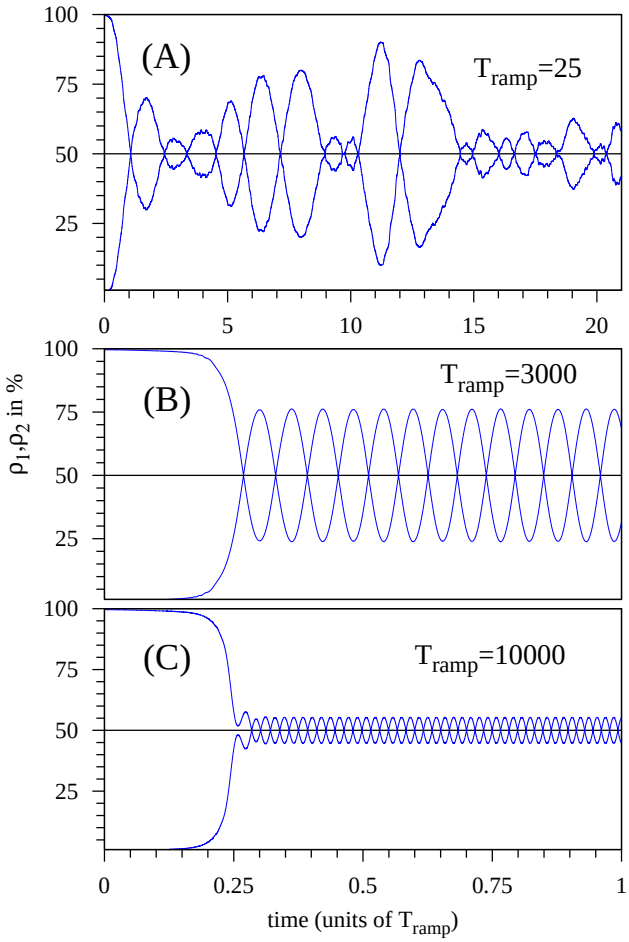

FIG. 2: (Color online) Quantifying how difficult it is to (fully) fragment a condensate. Plotted are the natural occupation numbers for $N = 200$ bosons (^{87}Rb atoms) with $\lambda_0 = 0.1$ and for three ramping-up times T_{ramp}. Increasing T_{ramp} the time-dependent many-body state approaches the ground-state of the double-well potential which is a (fully) fragmented BEC. Time is expressed in units of $\frac{mL^2}{\hbar} = 1.37$msec. For $T_{ramp} = 10000 = 13.7$sec which is of the order of a condensate's lifetime the amplitude of oscillations is still about 10%.

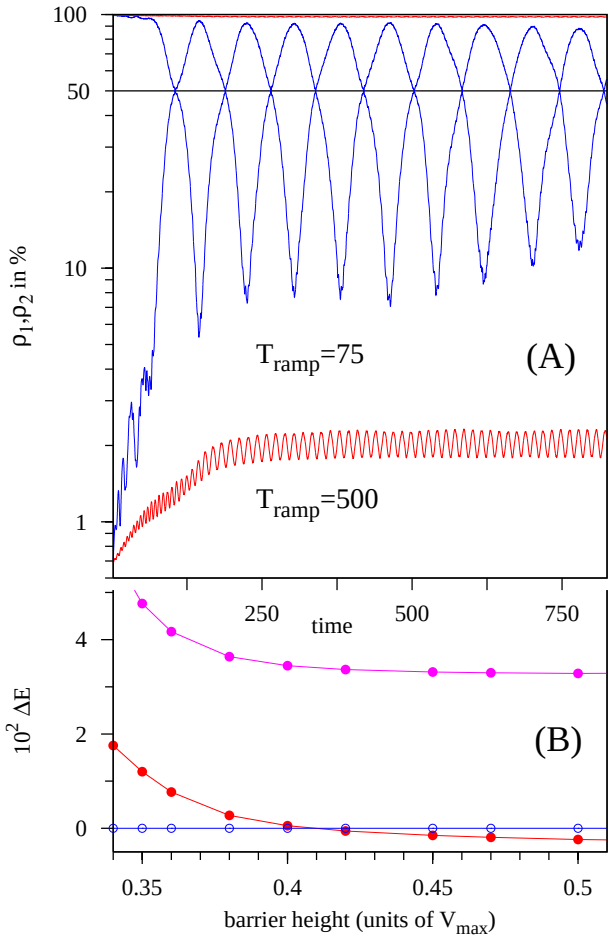

FIG. 3: (Color online) Same as in Fig. 1 except for the stronger interaction strength of $\lambda_0 = 0.3$. (A) For $T_{ramp} = 75$ the many-body wavefunction evolves from a condensed towards the two-fold fragmented ground state. For *longer* durations of the ramping-up, e.g., for $T_{ramp} = 500$, a 'counter-intuitive' regime is found in which the evolution of the condensate *is not* to the fragmented ground-state , but to a low-lying coherent excited state. (B) Static energy gaps ΔE as a function of barrier height. Around $V_{cr} \approx 0.41 V_{max}$ the condensed ground-state and lowest-excited fragmented state come very close to each other and interchange their order, see text for more details. Time is expressed in units of $\frac{mL^2}{\hbar} = 1.37$msec and energy in units of $\frac{\hbar^2}{mL^2} = 166$Hz.